

# Study of the ground-state energy of $^{40}\text{Ca}$ with the CD-Bonn nucleon-nucleon potential

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We have calculated the ground-state energy of the doubly-magic nucleus  $^{40}\text{Ca}$  within the framework of the Goldstone expansion using the CD-Bonn nucleon-nucleon potential. The short-range repulsion of this potential has been renormalized by integrating out its high-momentum components so as to derive a low-momentum potential  $V_{\text{low-k}}$  defined up to a cutoff momentum  $\Lambda$ . A simple criterion has been employed to establish a connection between this cutoff momentum and the size of the two-nucleon model space in the harmonic oscillator basis. This model-space truncation approach provides a reliable way to renormalize the free nucleon-nucleon potential preserving its many-body physics. The role of the  $3p-3h$  and  $4p-4h$  excitations in the description of the ground state of  $^{40}\text{Ca}$  is discussed.

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A fundamental goal of nuclear physics is to describe the properties of nuclei starting from the forces among nucleons. To this end, one has to employ many-body methods well suited to handle the strong short-range correlations that are induced in nuclei by the free-space nucleon-nucleon ( $NN$ ) potential  $V_{NN}$ . In other words, the method employed should produce results which are only slightly affected by the approximations involved, in the sense that it should be possible to keep the latter under control by way of convergence checks. This first-principle approach to the description of nuclear structure is nowadays referred to as *ab initio* approach [1].

In the last decade, thanks also to the considerable increase in computer power, a substantial progress has been achieved in microscopic approaches to the nuclear many-body problem, such as the Green's function Monte Carlo (GFMC) [2], no-core shell model (NCSM) [3, 4], and coupled-cluster methods (CCM) [5, 6].

Historically, the first calculations on light  $p$ -shell nuclei using the GFMC method were performed in the mid-1990s by the Argonne group [2]. They employed the high-precision  $NN$  potential  $AV18$  [7] plus a three-body interaction, the latter being fitted to reproduce the binding energy of selected few-body systems. Since then, these calculations have been successfully performed up to mass  $A = 12$  [8, 9], which is the present limit of GFMC with the available computer technology, owing to the exponential growth of the spin-isospin vector size [10]. This limit may be overcome by introducing effective interactions. In this way, the NCSM and CCM allow to perform calculations beyond the  $p$ -shell mass region. More precisely, the NCSM has been applied [3, 4] to nuclei with mass  $A \leq 16$ , using either coordinate-space or momentum dependent  $V_{NN}$ 's [11]. In some cases, also three-body interactions have been included [12, 13, 14]. The CCM can potentially be used for much heavier systems; in fact, in the late 1970s it was applied to the doubly-closed nuclei  $^{16}\text{O}$  and  $^{40}\text{Ca}$  [15]. Actually, coupled-cluster calculations em-

ploying modern  $V_{NN}$ 's [6] have been recently performed for valence systems around  $^{16}\text{O}$  [16, 17, 18]. CCM-like calculations are also those performed for nuclei up to  $^{16}\text{O}$  in Refs. [19, 20], where different realistic  $NN$  potentials have been used in the framework of the unitary model-operator approach (UMO) [5, 21, 22].

In Refs. [23, 24] a method to renormalize the bare  $NN$  interaction has been introduced, which may be considered an advantageous alternative to the use of the Brueckner  $G$  matrix. A low-momentum model space is defined up to a cutoff momentum  $\Lambda$ , and an effective low-momentum potential  $V_{\text{low-k}}$ , which satisfies the decoupling condition between the low- and high-momentum spaces, is derived from the original  $V_{NN}$ . The  $V_{\text{low-k}}$  is a smooth potential which preserves exactly the low-momentum on-shell properties of the original  $V_{NN}$  and can be used directly in nuclear structure calculations.

Recently, we have investigated [25, 26] how  $\Lambda$  is related to the dimension of the configuration space in the coordinate representation where our calculations are performed. We have introduced a simple criterion to map out the model space made up by the two-nucleon states in the harmonic-oscillator (HO) basis according to the value of the cutoff momentum  $\Lambda$ . The validity of this procedure was tested by calculating, in the framework of the Goldstone expansion, the ground-state (g.s.) energy of  $^4\text{He}$  with the CD-Bonn [27],  $\text{N}^3\text{LO}$  [28], and Bonn A [29] potentials, and comparing the results with those obtained using the Faddeev-Yakubovsky method. Taking into account perturbative contributions up to fourth order in  $V_{\text{low-k}}$ , we have found that the energy differences are at most 390 keV. The limited size of the discrepancies shows that this approach provides a reliable way to renormalize the  $NN$  potential preserving the physics beyond the two-body system too.

We also performed calculations for heavier systems, such as  $^{16}\text{O}$  and  $^{40}\text{Ca}$ , and obtained converged results for the CD-Bonn  $NN$  potential using a limited number

of oscillator quanta. As regards  $^{40}\text{Ca}$ , the g.s. energy was calculated including Goldstone diagrams only up to third order in  $V_{\text{low-k}}$ .

It seems fair to say that, at present, an *ab initio* calculation for  $^{40}\text{Ca}$  represents a major step on the way to the fully microscopic description of nuclear systems beyond  $^{16}\text{O}$ . In this work, we improve our calculation of the  $^{40}\text{Ca}$  g.s. energy including all the fourth-order contributions. A main motivation for this extension of our calculation of the g.s. energy of  $^{40}\text{Ca}$  is to study the role of a higher-order class of excitations, namely the  $3p-3h$  and  $4p-4h$  ones, which come into play starting from the fourth order of the Goldstone expansion. It should be pointed out that this is the first fully microscopic study of this nucleus, apart from a very preliminary calculation by Kumagai *et al.* [30] and Fujii *et al.* [20] in the framework of the unitary model-operator approach.

The first step of our calculation is to renormalize the short-range repulsion of the  $NN$  potential by integrating out its high momentum components through the so-called  $V_{\text{low-k}}$  approach (see Refs. [24, 31]). The low-momentum potential  $V_{\text{low-k}}$  preserves the physics of the two-nucleon system, and consequently the  $\chi^2/\text{datum}$  of the original  $NN$  potential, up to the cutoff momentum  $\Lambda$ . As mentioned above, it is a smooth potential and can therefore be used directly in a perturbative nuclear structure calculation.

The  $V_{\text{low-k}}$  is defined in the momentum space, and it is desirable to relate the cutoff momentum  $\Lambda$  to the size of the harmonic-oscillator (HO) space in the coordinate representation [25, 26], where we perform our calculations for finite nuclei.

Let us consider the relative motion of two nucleons in a HO well in the momentum representation. For a given maximum relative momentum  $\Lambda$ , the corresponding maximum value of the energy is:

$$E_{\text{max}} = \frac{\hbar^2 \Lambda^2}{M} , \quad (1)$$

where  $M$  is the nucleon mass.

This relation may be rewritten in terms of the maximum number  $N_{\text{max}}$  of HO quanta in the relative coordinate system. For a given HO parameter  $\hbar\omega$  we have:

$$\left(N_{\text{max}} + \frac{3}{2}\right) \hbar\omega = \frac{\hbar^2 \Lambda^2}{M} . \quad (2)$$

The above equation provides a simple criterion to map out the two-nucleon HO model space. If we write the two-nucleon states as the product of HO wave functions

$$|a\ b\rangle = |n_a l_a j_a, n_b l_b j_b\rangle , \quad (3)$$

our HO model space is defined as spanned by those two-nucleon states that satisfy the constraint

$$2n_a + l_a + 2n_b + l_b \leq N_{\text{max}} . \quad (4)$$

Making use of the above approach, in this paper we have studied the g.s. energy of  $^{40}\text{Ca}$  within the framework of the Goldstone expansion [32]. We start from the purely intrinsic hamiltonian

$$H = \left(1 - \frac{1}{A}\right) \sum_{i=1}^A \frac{p_i^2}{2M} + \sum_{i<j} \left(V_{ij} - \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{MA}\right) , \quad (5)$$

where  $V_{ij}$  stands for the renormalized  $V_{NN}$  potential plus the Coulomb force, and construct the Hartree-Fock (HF) basis expanding the HF single particle (SP) states in terms of HO wave functions. The next step is to sum up all the Goldstone linked diagrams for the ground-state energy up to fourth-order in the two-body interaction. The complete list of the fourth-order diagrams can be found in Ref. [33, 34]. Using Padé approximants [33, 35] one may obtain a value to which the perturbation series should converge. In this work, we report results obtained using the Padé approximant [2|2], whose explicit expression is

$$[2|2] = \frac{E_0(1 + \gamma_1 + \gamma_2) + E_1(1 + \gamma_2) + E_2}{1 + \gamma_1 + \gamma_2} , \quad (6)$$

where

$$\gamma_1 = \frac{E_2 E_4 - E_3^2}{E_1 E_3 - E_2^2} , \quad \gamma_2 = -\frac{E_3 + E_1 \gamma_1}{E_2} ,$$

$E_i$  being the  $i$ th order energy contribution in the Goldstone expansion.

In principle, our results should not depend on the HO parameter  $\hbar\omega$ , whose value characterizes the HO wavefunctions employed to expand the HF SP states. Actually, our calculations are made in a truncated model space, whose size is related to the values of the cutoff momentum  $\Lambda$  and the  $\hbar\omega$  parameter by relations (2) and (4). Obviously, for  $N_{\text{max}} \rightarrow \infty$  this dependence disappears. So, we perform our calculations increasing the  $N_{\text{max}}$  value (and consequently  $\Lambda$ ) for different  $\hbar\omega$  values. Finally, we choose the results which correspond to the value of  $\hbar\omega$  for which they are practically independent of  $N_{\text{max}}$ .

In Fig. 1 we report the ground-state energy of  $^{40}\text{Ca}$  calculated with the CD-Bonn potential [27]. The straight red line indicates the experimental datum [36] while the other curves represent our calculated values, for different values of  $\hbar\omega$ , versus the maximum number of HO quanta  $N_{\text{max}}$  that limits the two-nucleon configurations according to relation (4).

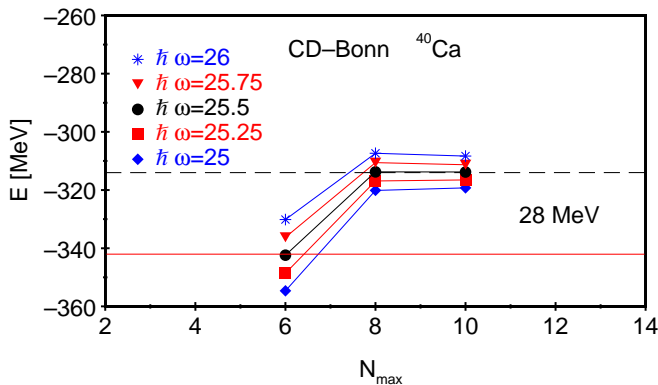


FIG. 1: (Color online) Ground-state energy of  $^{40}\text{Ca}$  with the CD-Bonn potential as a function of  $N_{\text{max}}$ , for different values of  $\hbar\omega$ . The straight line represents the experimental value, while the dashed one our converged result. The value of the energy difference between the former and the latter is also reported.

We obtain convergence for  $\hbar\omega = 25.5$  MeV, and the corresponding energy is  $(-314 \pm 3)$  MeV, as indicated in Fig. 1 by the dashed line. The error has been evaluated taking into account the dependence of our results on  $\hbar\omega$  [26]. In Ref. [25] we calculated the  $^{40}\text{Ca}$  g.s. energy taking into account all the contributions in the Goldstone expansion up to third order. The converged value, obtained with the Padé approximant [2/1] turned out to be  $(-308 \pm 3)$  MeV with  $\hbar\omega = 25.5$  MeV. The difference between the two results is only about 2% of the total binding energy, the converged value at fourth order being 6 MeV more attractive than the third-order one. This is in line with the outcome of our calculations [25, 26] of the g.s. energy of  $^4\text{He}$  and  $^{16}\text{O}$  with the CD-Bonn potential. In those cases the converged fourth-order result was 0.6 MeV and 3 MeV more attractive, respectively, than the converged third-order one.

TABLE I: Calculated  $2p-2h$ ,  $3p-3h$ , and  $4p-4h$  fourth-order contributions (in MeV) to the g.s. energy of  $^{40}\text{Ca}$  with the CD-Bonn potential. Calculations correspond to  $N_{\text{max}} = 10$ .

Nucleus	$2p-2h$	$3p-3h$	$4p-4h$	4th order
$^{40}\text{Ca}$	-15	-16	+24	-7

It is worth now to make a brief discussion about the role of  $3p-3h$  and  $4p-4h$  contributions which, as pointed out before, come into play only at the fourth order of the Goldstone expansion and beyond. To this end, we report in Table I the  $2p-2h$ ,  $3p-3h$ , and  $4p-4h$  fourth-order contributions to the g.s. energy of  $^{40}\text{Ca}$  with the CD-Bonn potential. Since we use the Hartree-Fock basis, all  $1p-1h$  excitations of the ground state are identically zero. The inspection of Table I evidences that the role played by the  $3p-3h$  and  $4p-4h$  excitations is significant, their net repulsive contribution being 8 MeV. The latter counterbalances the fourth-order contribution of the  $2p-2h$  excitations, so that the total fourth-order contribution is only -7 MeV.

As regards the comparison with experiment, our calculated  $^{40}\text{Ca}$  binding energy underestimates the experimental one by 28 MeV, which is 8% of the experimental binding energy. Our calculations of  $^4\text{He}$  and  $^{16}\text{O}$  with the CD-Bonn potential [25, 26] show the same percent difference from the experimental data. This seems to confirm the need of a three-body force in addition to the  $NN$  CD-Bonn potential, in order to compensate for the lack of attraction of the latter.

In conclusion, this work presents a fully microscopic calculation of the ground-state energy of  $^{40}\text{Ca}$  with the CD-Bonn  $NN$  potential. We hope that this may stimulate, and provide some useful hints to, future non-perturbative *ab initio* calculations.

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